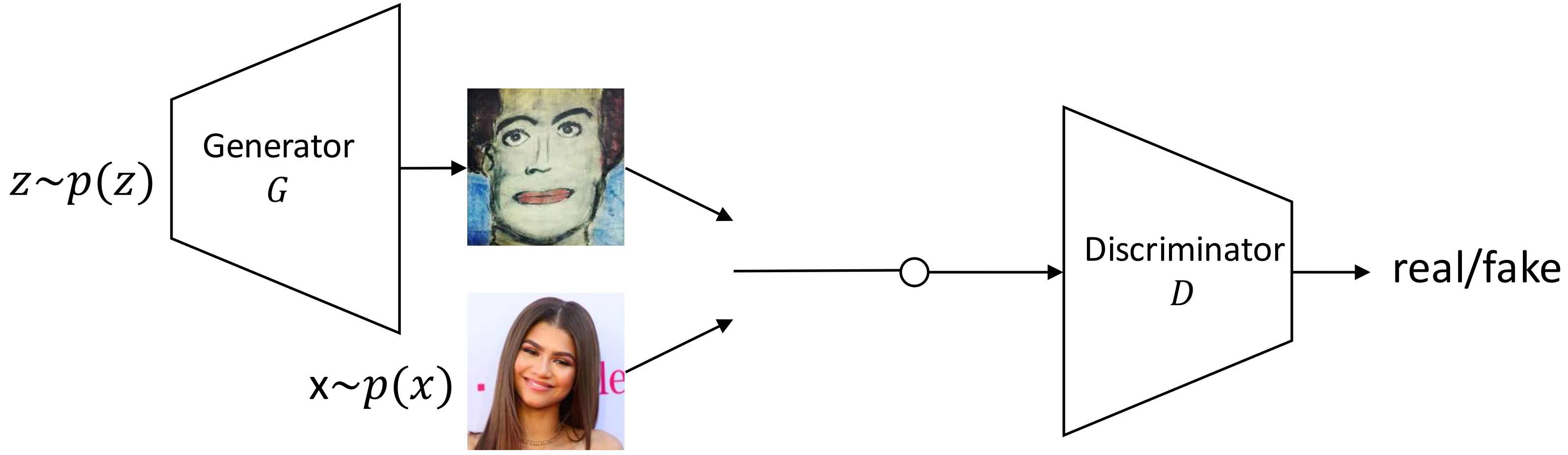
Normalizing Flows/ Invertible Models

Lecture 7

18-789

Recap: Generative Adversarial Networks



In practice, we update G/D alternatingly!

$$\min_G \max_D E_{x\sim p(x)}[\log D(x)] + E_{z\sim p(z)}[\log(1 - D(G(z)))]$$

Generated sample

Discriminator tries to classify real vs fake

Generator tries to fool the discriminator

Recap: Theory of GAN

- For a fixed generator G (with parameter θ), the optimal discriminator is

$$D^*(x) = \frac{p(x)}{p(x) + p_\theta(x)}$$

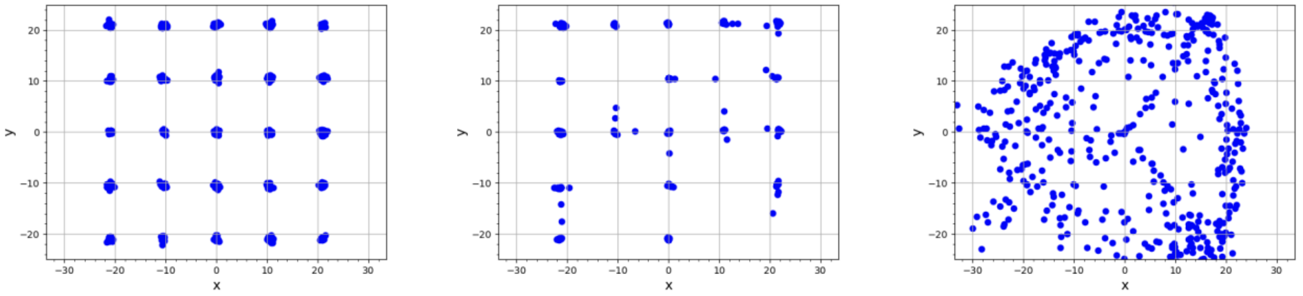
- Assuming optimal discriminator, the generator is trained to minimize JSD (Jenson-Shannon Divergence)

$$\mathcal{L}(G) = 2\mathrm{JSD}(p(x)|p_\theta(x)) - \log 4$$

$$\min_G \max_D E_{x\sim p(x)}[\log D(x)] + E_{z\sim p(z)}[\log(1 - D(G(z)))]$$

Recap: Wasserstein GAN

- Motivation: JSD is constant when two distributions have non-overlapped support
- Solution: Wasserstein distance
  - $$W(p, p_\theta) = \inf_{\gamma \in \Pi(p, p_\theta)} E_{(x,y)\sim\gamma}[\ ||x-y||\ ]$$
    $$= \sup_{||D||_L \leq 1} E_{x\sim p}[D(x)] - E_{x\sim p_\theta}[D(x)]$$
- Empirical results not very good
- Lesson: GANs do not really minimize a specific divergence



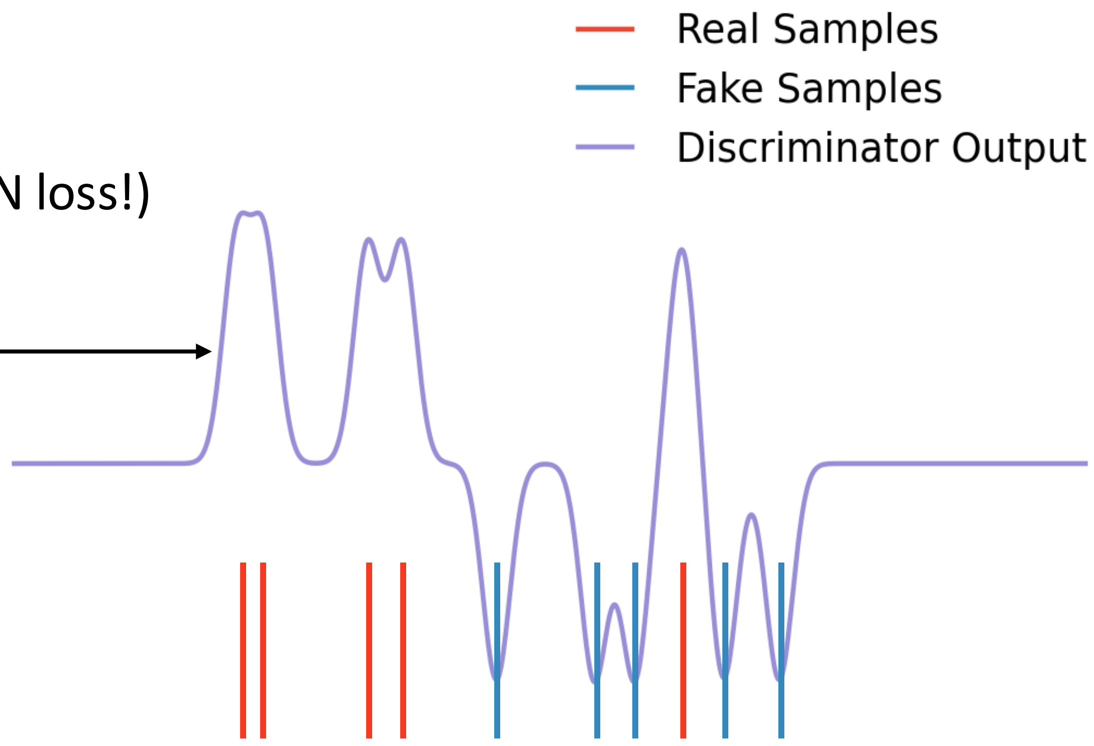
(a) True data (b) GAN (d) WGAN

Recap: Improving Stability of Training GANs

- Key: prevent discriminator overfitting
  - Data augmentation
  - Lipschitz continuity
    - Gradient Penalty (can be applied on any GAN loss!)
    - Spectral Normalization

$$\frac{|f(x) - f(y)|}{|x - y|} \leq K, \forall x, y$$

Large Lipschitz constant around "spikes"!



Recap: Improving Stability of Training GANs

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- Other tricks:
  - Adam $\beta_1 = 0$ for G&D (No momentum)

$$m_w^{(t+1)} := \beta_1 m_w^{(t)} + (1 - \beta_1) \nabla_w L^{(t)}$$

$$w^{(t+1)} := w^{(t)} - \eta \frac{\hat{m}_w}{\sqrt{\hat{v}_w} + \varepsilon}$$

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    - Adam $\beta_1 = 0$ for G&D (No momentum)
    - Exponential Moving Average for G

$$\theta_{EMA}^{(t)} = \beta\theta_{EMA}^{(t-1)} + (1-\beta)\theta^{(t)}$$

"The Unusual Effectiveness of Averaging in GAN Training", Yazıcı et al., ICLR 2019

Recap: Improving Stability of Training GANs

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- Other tricks:
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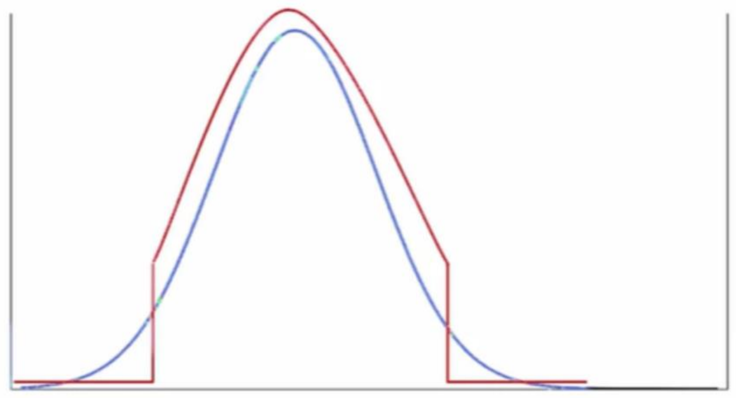
  - Exponential Moving Average for G
  - Truncation trick for G

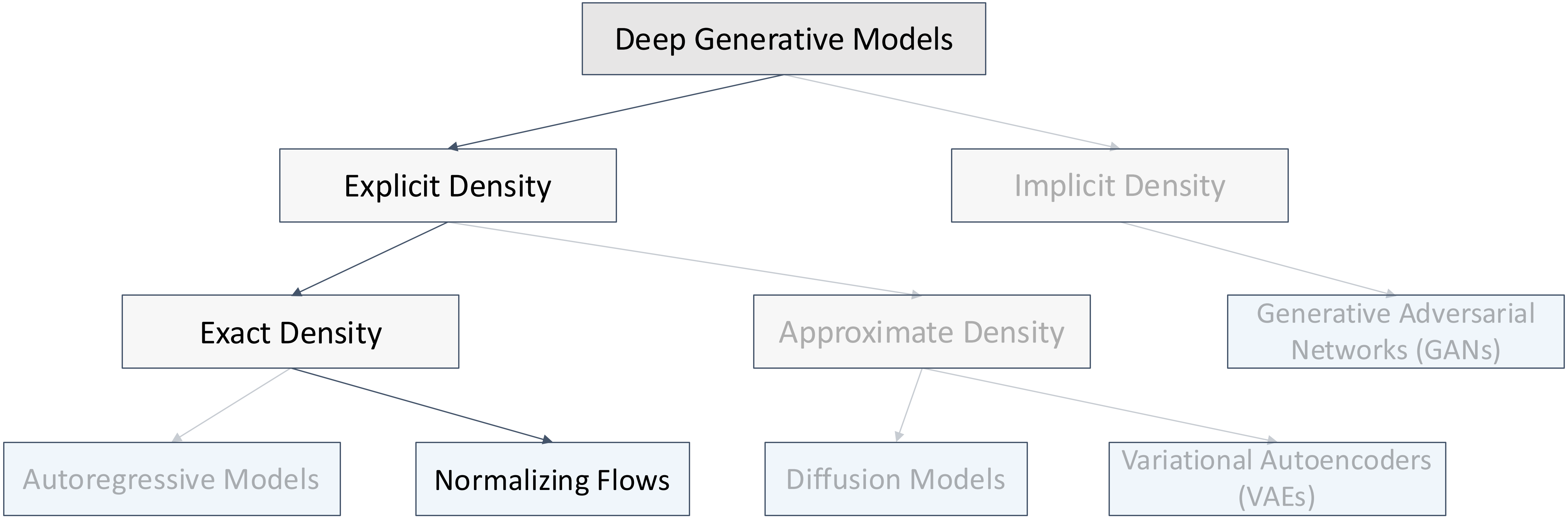


“Large Scale GAN Training for High Fidelity Natural Image Synthesis”, Brock et al., ICLR 2019

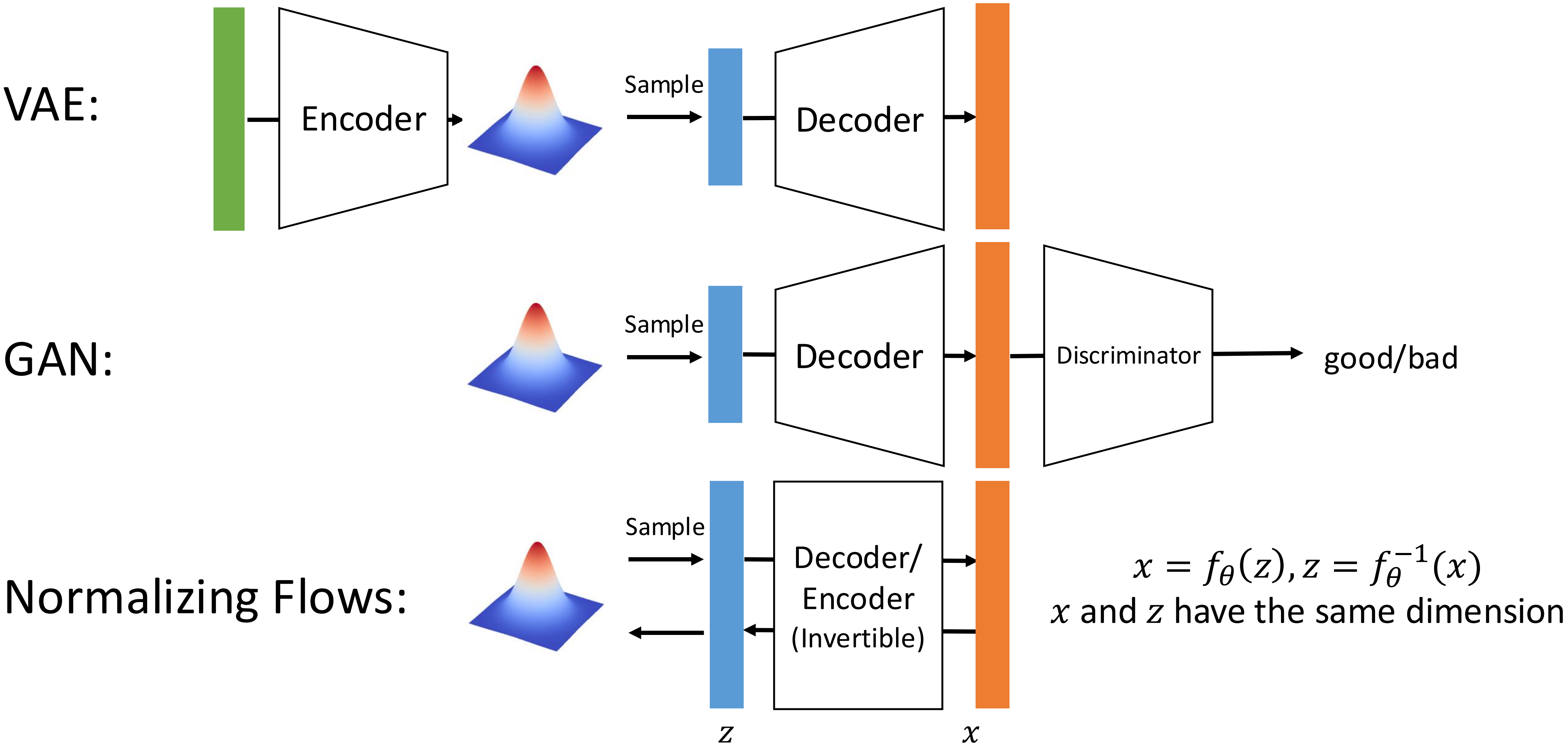
Deep Generative Models (so far)

- Autoregressive Models: Generation not parallelizable
- VAE: Blurry
- GAN: Unstable training
- Normalizing Flows: Stable training, parallelized and sharp generation

Normalizing Flows

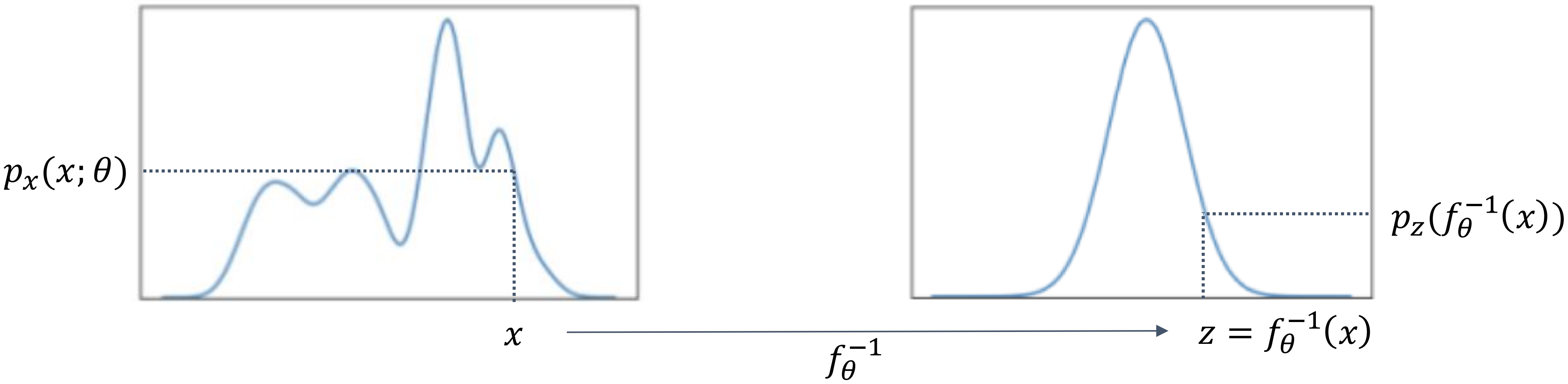


Normalizing Flows



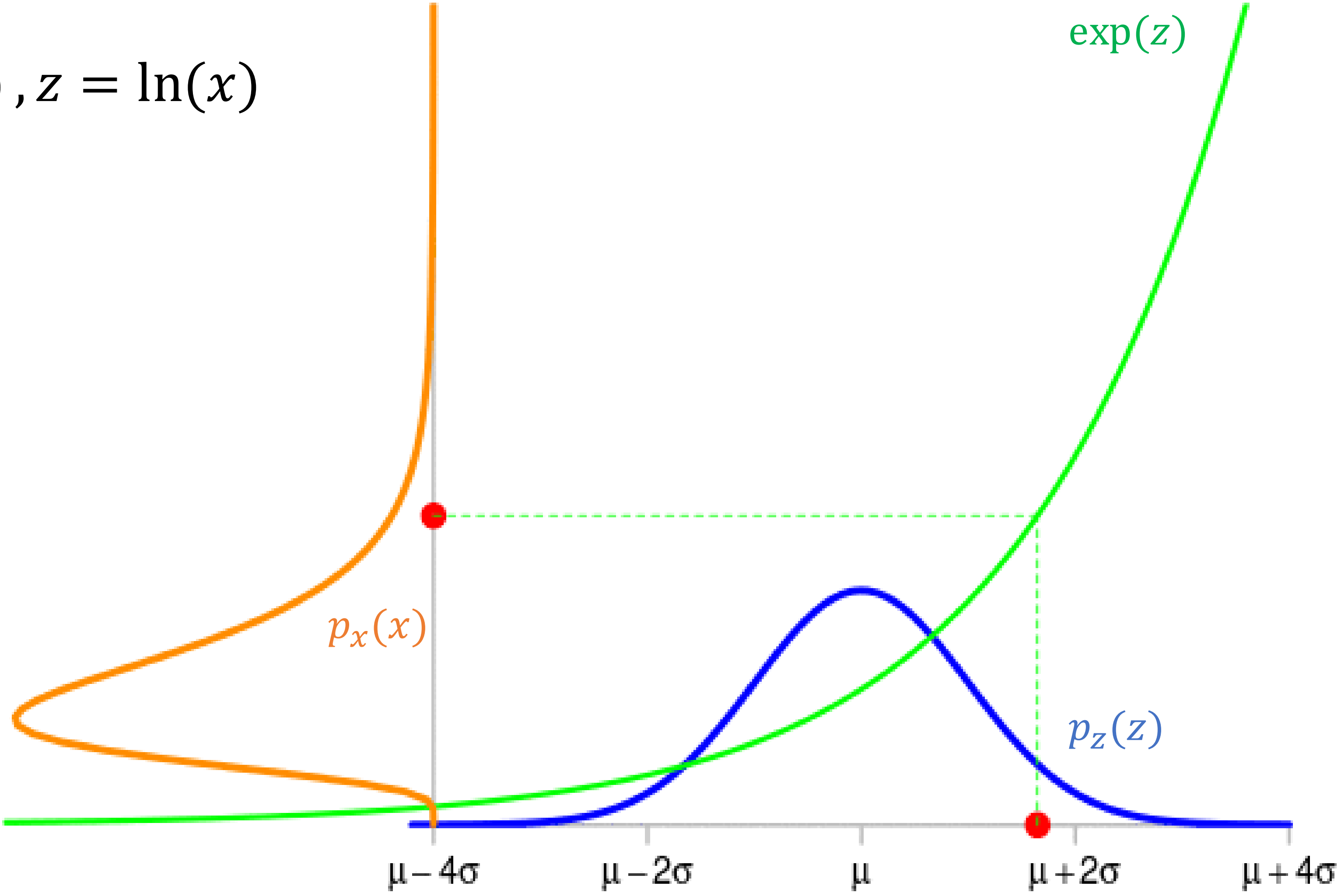
Change of Variables Theorem

- $x = f_\theta(z), z = f_\theta^{-1}(x)$
- $\boxed{p_x(x;\theta) = \underbrace{p_z(f_\theta^{-1}(x))}_{\text{Density of the encoded } z \text{ under the prior}} \underbrace{\left|\det \frac{\partial f_\theta^{-1}(x)}{\partial x}\right|}_{\text{Jacobian determinant of } f_\theta^{-1} \text{ (For 1D: simply the derivative of } f_\theta^{-1}\text{)}}}$



Change of Variables: Intuition

- $x = \exp(z) \, , z = \ln(x)$



Source: stlaPblog, “The change of variables of formula for probability density functions”

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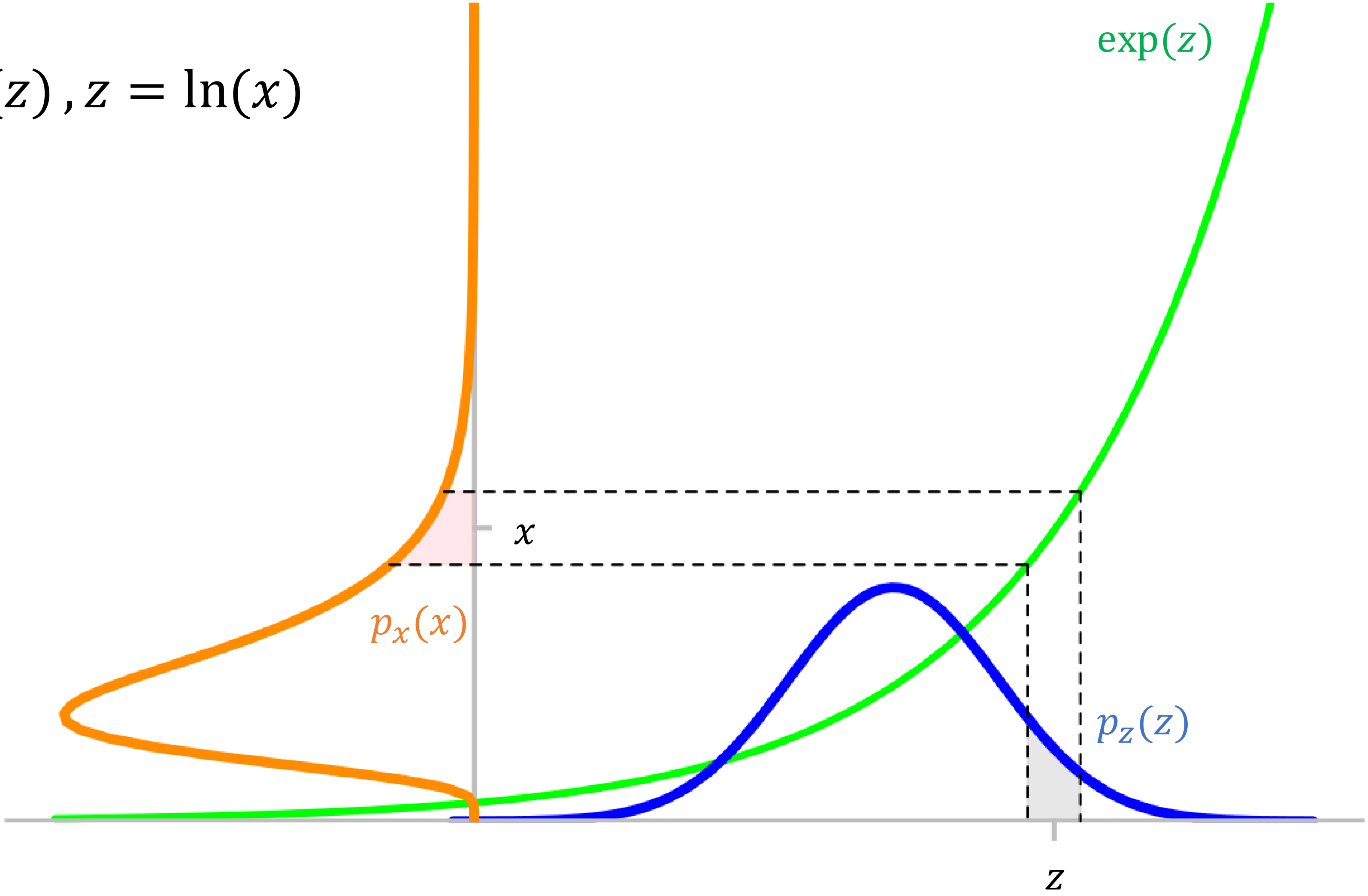
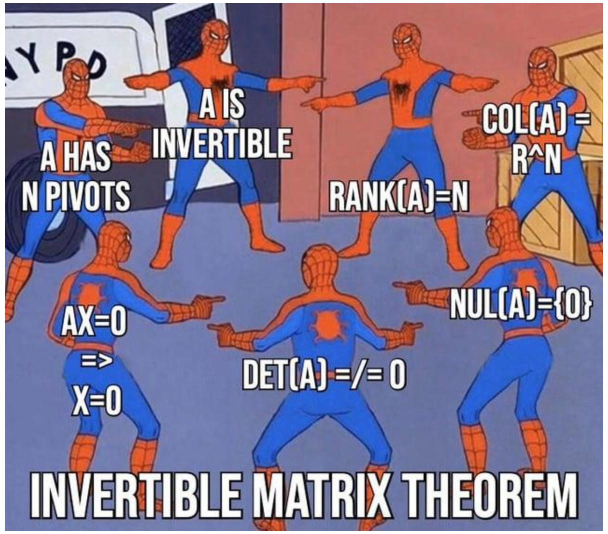


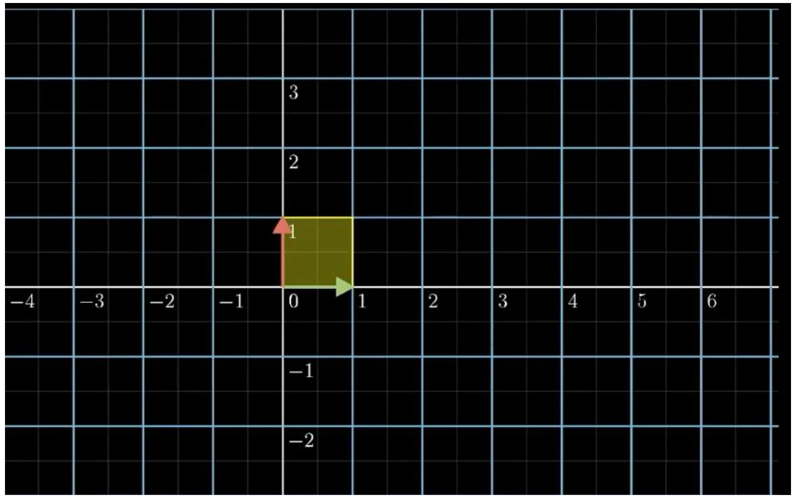
Source: stlaPblog, "The change of variables of formula for probability density functions"

Jacobian Determinant $p_x(x;\theta) = p_z(f_\theta^{-1}(x)) \left|\det \frac{\partial f_\theta^{-1}(x)}{\partial x}\right|$

- Jacobian matrix: Local linear approximation of f (around x)
- Jacobian *Determinant*: How much does f "stretches" (> 1) or "compresses" (< 1) space (around x)
  - Example: $\mathcal{J} = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}$
  - What's the determinant of $\mathcal{J}$?
- $\det \mathcal{J} \neq 0 \Leftrightarrow \mathcal{J}$ is invertible

$$\mathbf{J} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

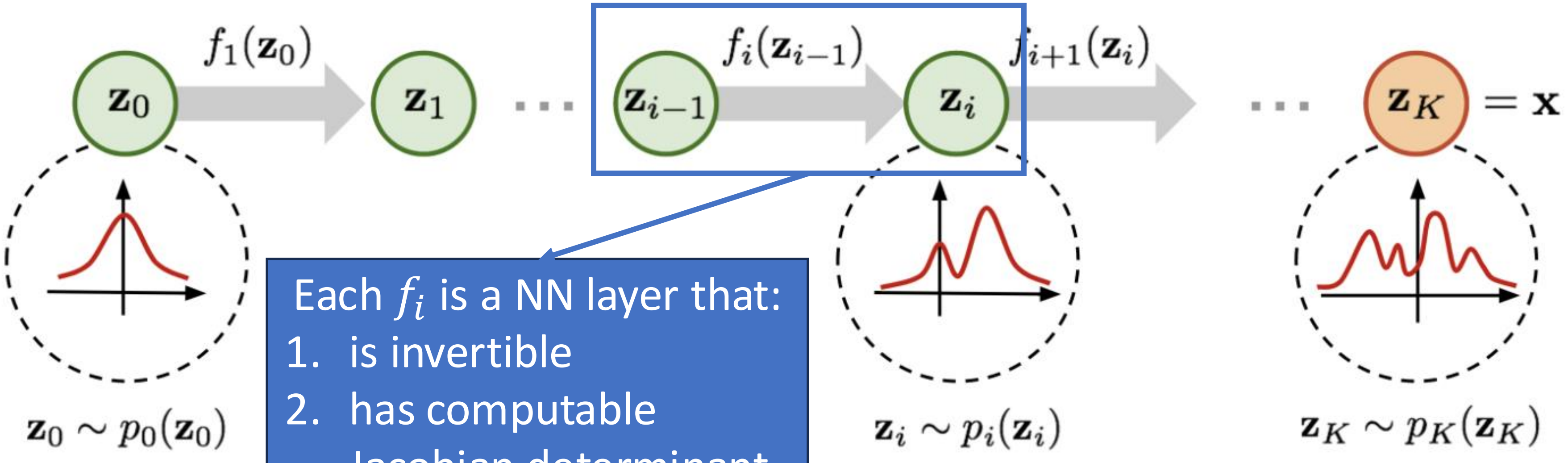




Source: Khan Academy, "The Jacobian Determinant"

Normalizing Flows

- Normalizing Flows: a **sequence** of K invertible transformation
  - $f = f_K \circ f_{K-1} \circ \cdots \circ f_2 \circ f_1$
- $p_x(x;\theta) = p_z\left(f_\theta^{-1}(x)\right) \prod_{i=1}^{K} \left|\det \frac{\partial f_i^{-1}}{\partial z_i}\right| = p_z\left(f_\theta^{-1}(x)\right) \prod_{i=1}^{K} \left|\det \frac{\partial f_i}{\partial z_{i-1}}\right|^{-1}$
- $\log p_x(x;\theta) =$

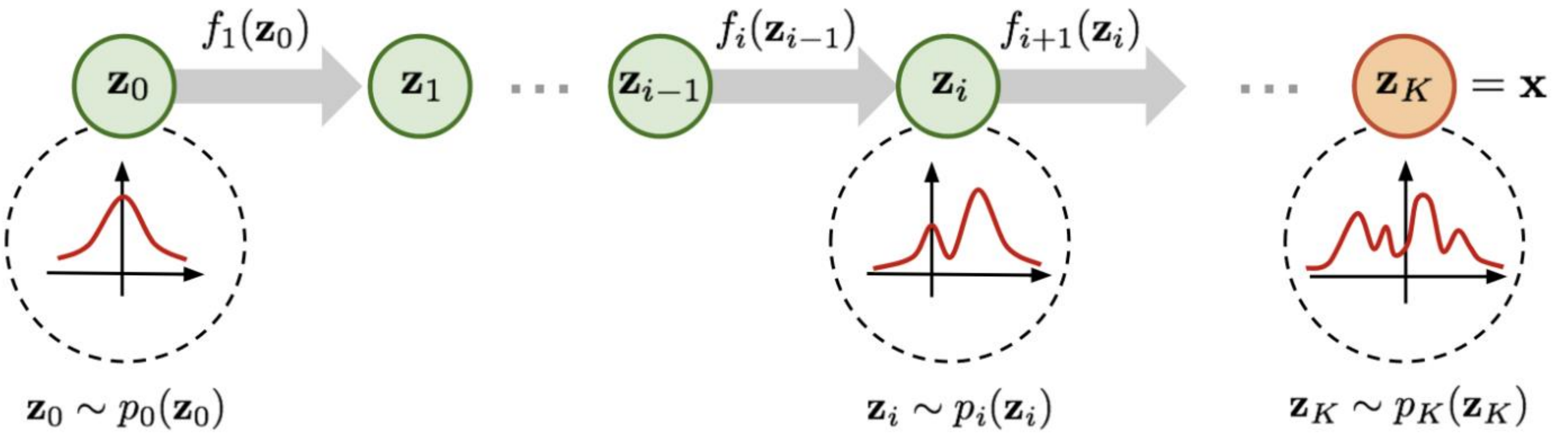


Each f_i is a NN layer that:
1. is invertible
2. has computable Jacobian determinant

Source: Lilian Weng, "Flow-based Deep Generative Models"

Normalizing Flows

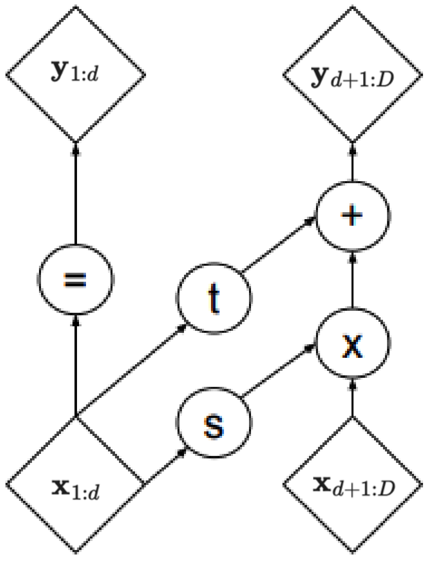
1. How to model the joint distribution of high-dimensional data?
   - $p_\theta(x)$: $x = f_{\theta_K} \circ f_{\theta_{K-1}} \circ \cdots \circ f_{\theta_2} \circ f_{\theta_1}(z)$, where z is the same dimension as x
   - $p(z) = N(0, I)$ is standard Gaussian
2. How to optimize your model?
   - Maximize Likelihood



Example: affine coupling layer

Each f_i is a NN layer that:
1. is invertible
2. has computable Jacobian determinant

- Split the input along certain dimension (e.g. channel)
  - The first part stays the same
  - The second part undergoes an affine transformation and both scale and shift parameters are predicted by the first part with an FC layer

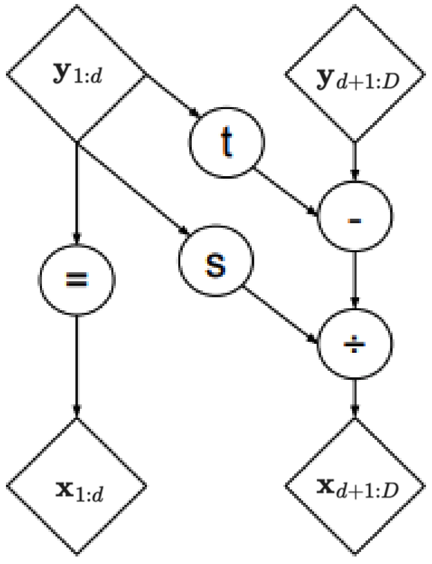


(a) Forward propagation

$$
\begin{aligned}
\mathbf{y}_{1:d} &= \mathbf{x}_{1:d} \\
\mathbf{y}_{d+1:D} &= \mathbf{x}_{d+1:D} \odot \exp(s(\mathbf{x}_{1:d})) + t(\mathbf{x}_{1:d})
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{x}_{1:d} &= \mathbf{y}_{1:d} \\
\mathbf{x}_{d+1:D} &= (\mathbf{y}_{d+1:D} - t(\mathbf{y}_{1:d})) \odot \exp(-s(\mathbf{y}_{1:d}))
\end{aligned}
$$

$$
\mathbf{J} = \begin{bmatrix} \mathbb{I}_d & \mathbf{0}_{d\times(D-d)} \\ \frac{\partial \mathbf{y}_{d+1:D}}{\partial \mathbf{x}_{1:d}} & \operatorname{diag}(\exp(s(\mathbf{x}_{1:d}))) \end{bmatrix}
$$



(b) Inverse propagation

[1] "Density estimation using Real NVP", Dinh et al., 2016

Think-pair-share:

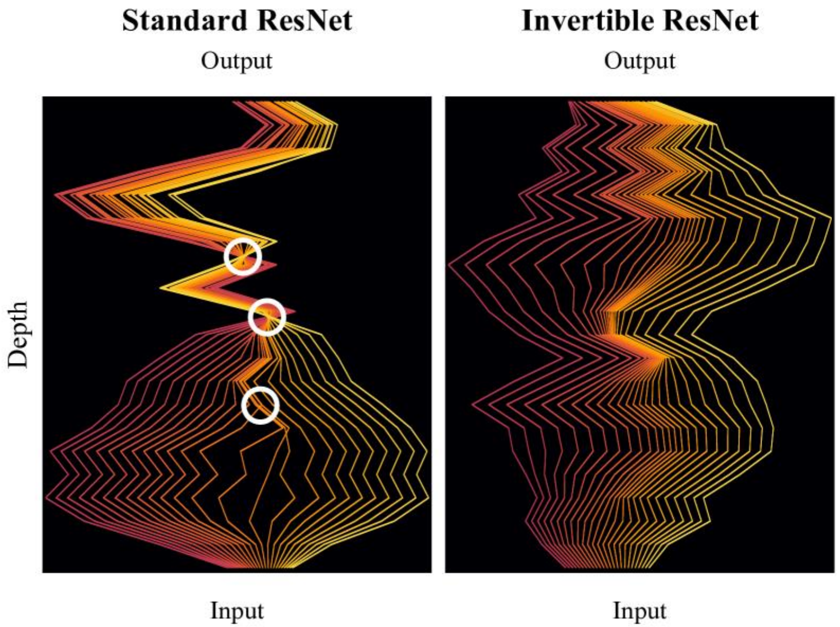
- Given 2D input and an affine coupling layer defined as follows:

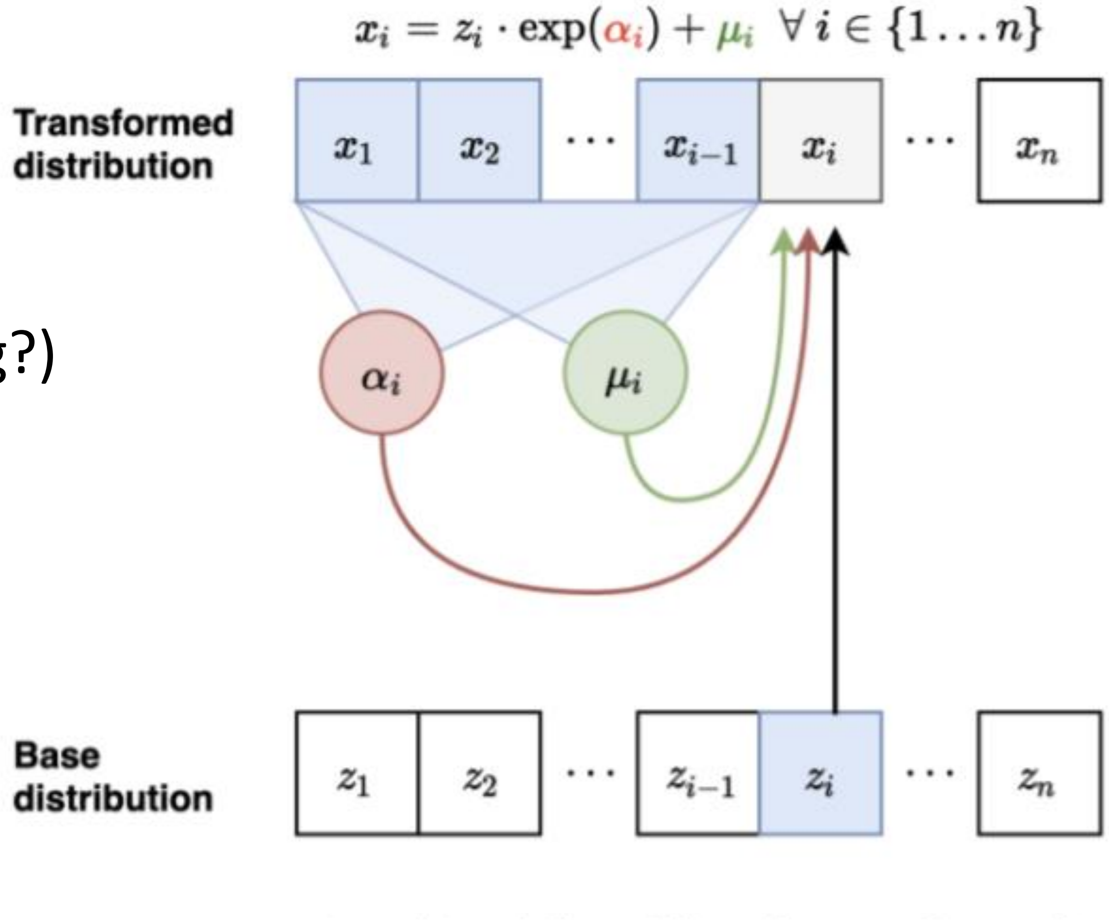
  $$\begin{cases} y_1 = x_1 \\ y_2 = x_2 \exp\big(s(x_1)\big) + t(x_1) \end{cases}$$

  where $s(x_1) = 0.5x_1 - 1, t(x_1) = 2x_1 + 1$
- Q1: Given input $(x_1, x_2) = (2, 3)$
  - compute output (y_1, y_2)
  - What's the Jacobian determinant?
- Q2: Given output $(y_1, y_2) = (0, 1)$
  - compute input (x_1, x_2)

Other invertible layers

- Permutation [1]
- Autoregressive Flow [2] (vs. affine coupling?)
- Invertible convolution [3]
- Invertible Residual Networks [4]





Inference

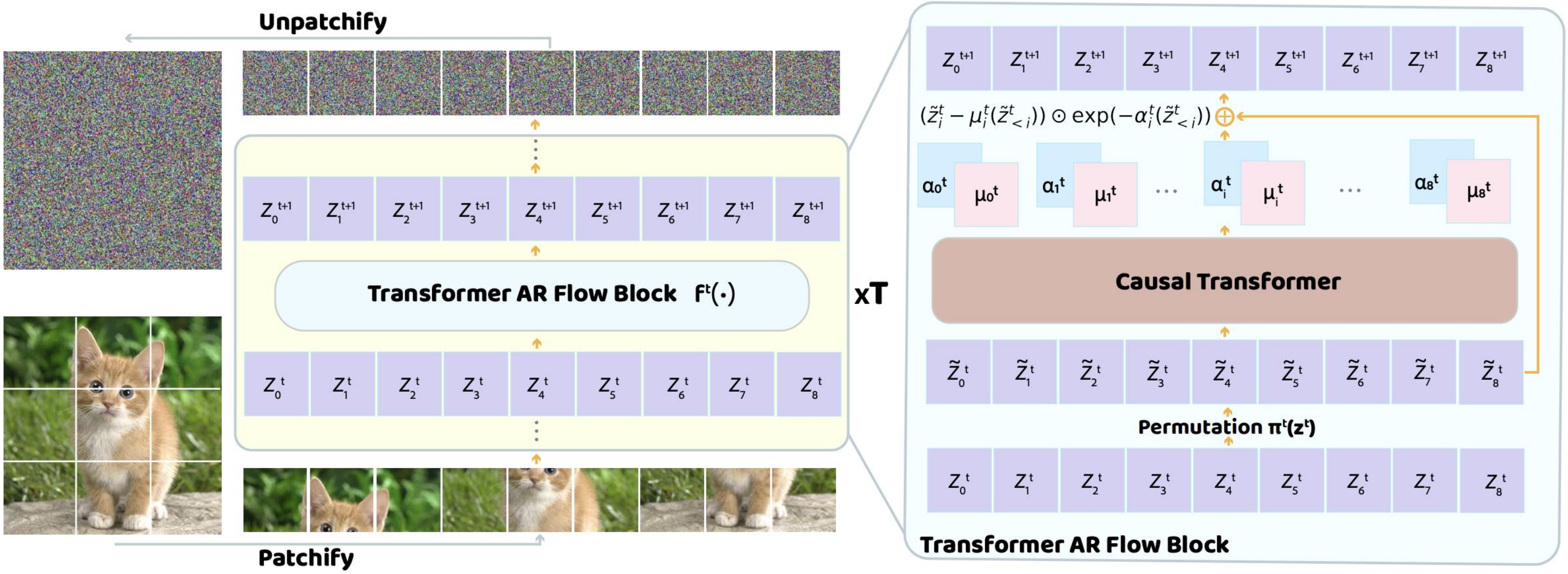
[1] “Density estimation using Real NVP”, Dinh et al., 2016
[2] “Masked Autoregressive Flow for Density Estimation”, Papamakarios et al., 2017
[3] “Glow: Generative Flow with Invertible 1x1 Convolutions”, Kingma et al., 2018
[4] “Invertible Residual Networks”, Behrmann et al., 2019

How do Normalizing Flows perform?

Glow, 2018 (Normalizing Flows)

StyleGAN, 2019 (GANs)

Modern Normalizing Flows



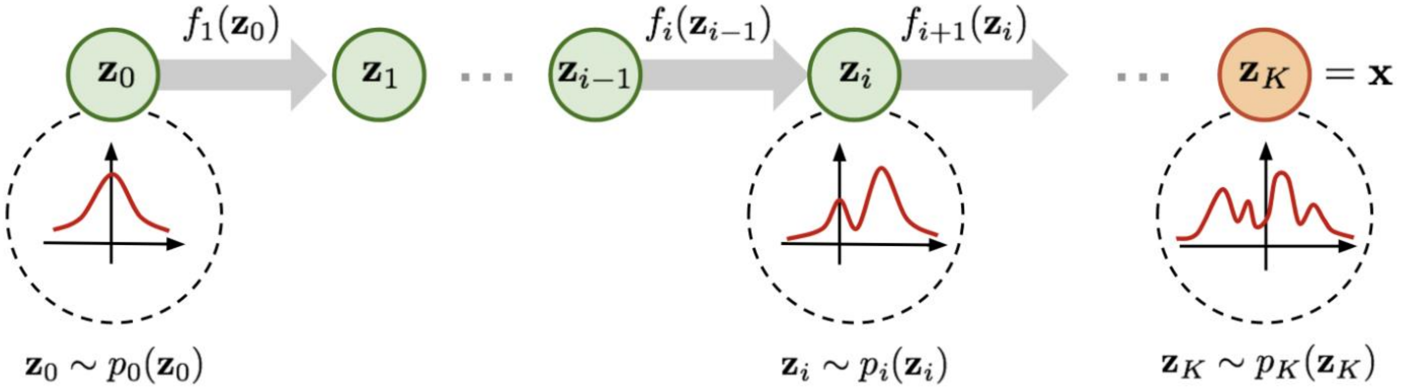
“Normalizing Flows are Capable Generative Models”, Zhai et al., 2024

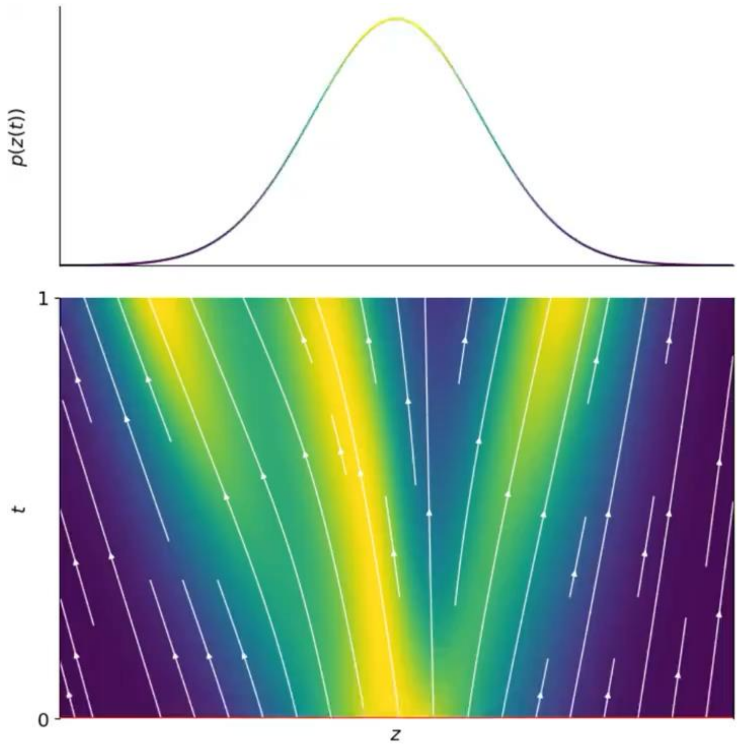
Modern Normalizing Flows

"Normalizing Flows are Capable Generative Models", Zhai et al., 2024

Continuous Normalizing Flows (CNFs)

- Normalizing Flows consist of K discrete transformations
  - $z_i = f_i(z_{i-1}),\ z_K = f_K \circ f_{K-1} \circ \cdots \circ f_2 \circ f_1(z_0)$
- Generalize to continuous case
  - $\frac{\partial z}{\partial t} = f(z_t, t), 0 < t < 1$
  - $z_{t+\Delta t} \approx f(z_t, t)\Delta t + z_t,\ z_1 = z_0 + \int_0^1 f(z_t, t)\, dt$





"Neural Ordinary Differential Equations", Chen et al., 2018

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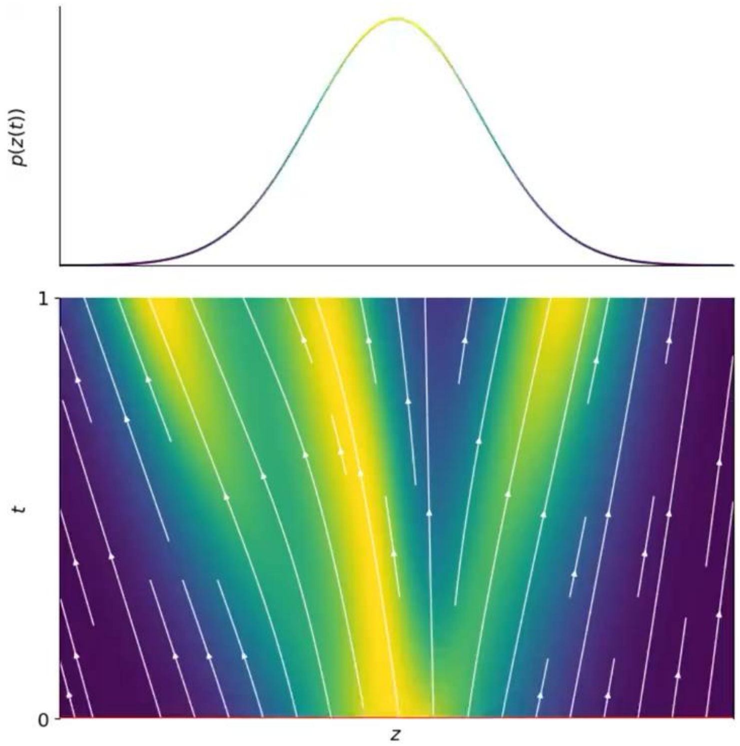
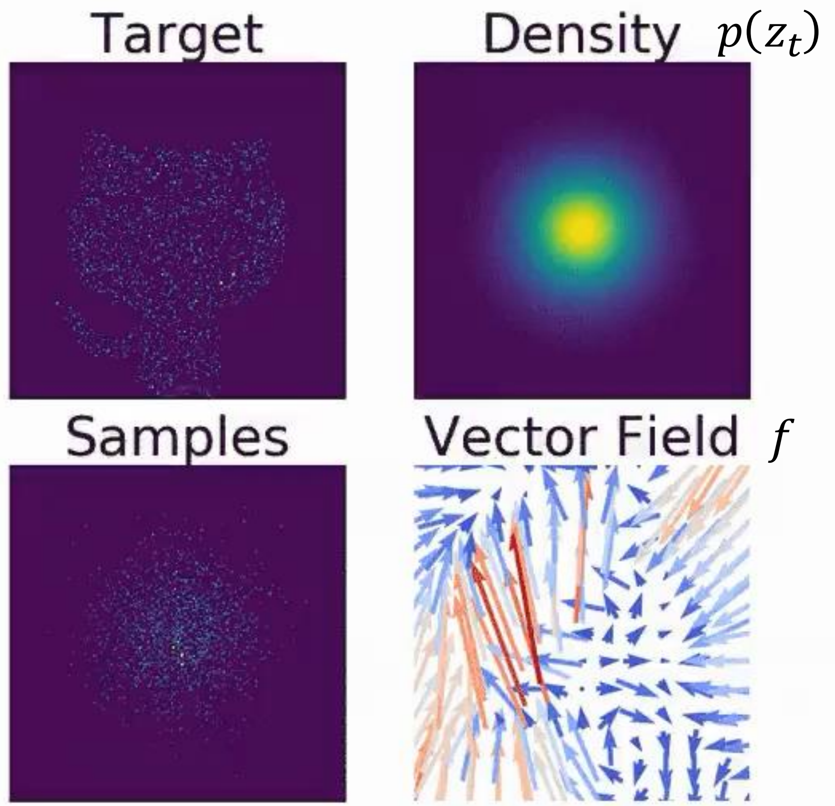
- Training objective
  - $\log p(z_1) = \log p(z_0) - \int_0^1 \mathrm{Trace}\left(\frac{\partial f}{\partial z_t}\right) dt$
  - Assume z_0 is noise and z_1 is data



"Neural Ordinary Differential Equations", Chen et al., 2018

Continuous Normalizing Flows (CNFs)

- Network
  - A neural network $f(z_t, t)$ conditioned on data z_t and time t
  - Unrestricted architecture
- Training
  - $\log p(z_1) = \log p(z_0) - \int_0^1 \mathrm{Trace}\left(\frac{\partial f}{\partial z_t}\right) dt$
  - Solve the forward **ODE** to compute log-likelihood
    - Find the latent $z_0 = z_1 + \int_1^0 f(z_t, t)\, dt$
    - Estimate the trace $\int_0^1 \mathrm{Trace}\left(\frac{\partial f}{\partial z_t}\right) dt$
  - Backpropagate through the **ODE**
- Sampling
  - Solve the backward **ODE**
  - $z_1 = z_0 + \int_0^1 f(z_t, t)\, dt$



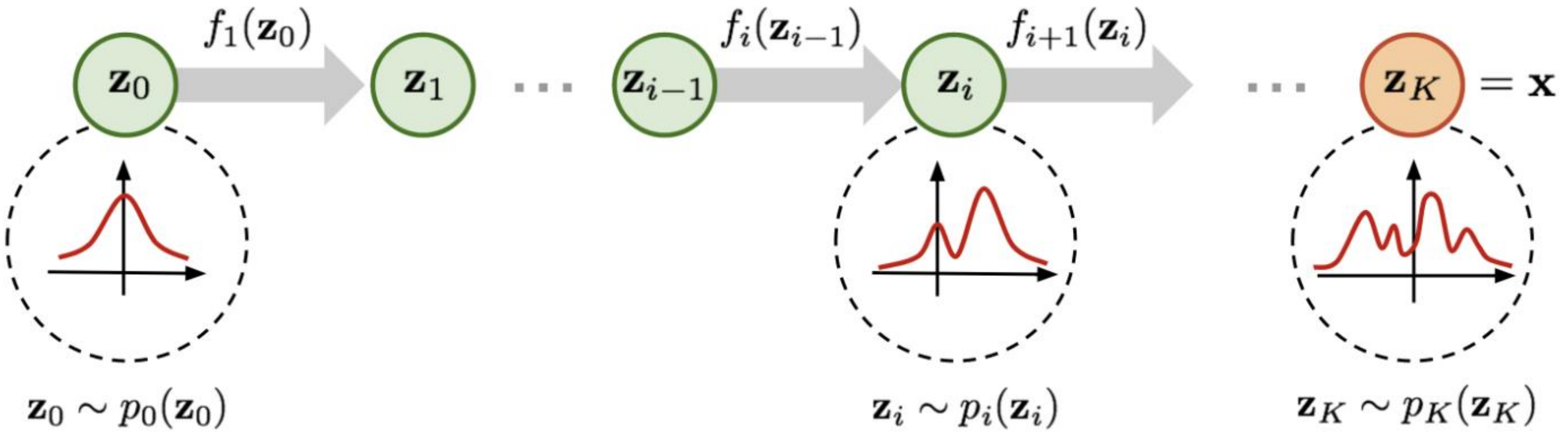
Pros and Cons

- (Discrete) Normalizing Flows
  - Different parameters at different steps
  - Restricted (invertible) architecture
- Continuous Normalizing Flows
  - Same parameters at different steps
  - Unrestricted architecture

Diffusion is a CNF at inference time! (but trained in a more efficient way)

Small f (e.g., single layer) -> not expressive

Large f (e.g., a large network) -> slow training



5 Minute Quiz

- On Canvas
- Passcode: snail